Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:38 AM GMT

PDB ID	:	2XQR
Title	:	CRYSTAL STRUCTURE OF PLANT CELL WALL INVERTASE IN COMPLEX WITH A SPECIFIC PROTEIN INHIBITOR
Authors	:	Hothorn, M.; Van Den Ende, W.; Lammens, W.; Rybin, V.; Scheffzek, K.
Deposited on	:	2010-09-07
Resolution	:	2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

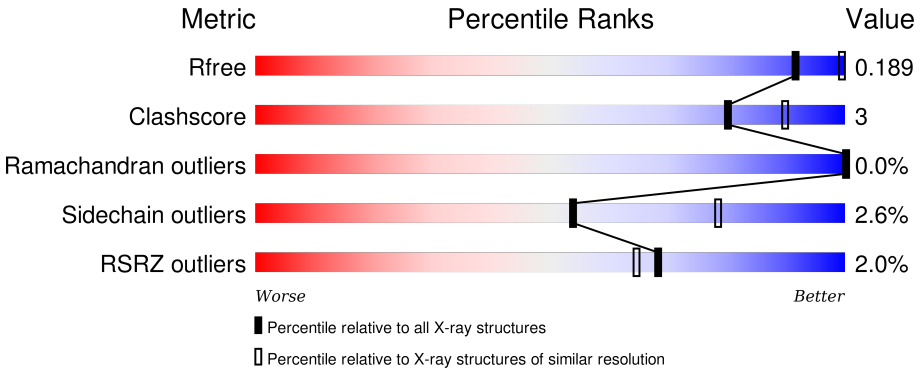
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	537	90% 9%
1	C	537	90% 10%
1	E	537	89% 11%
1	G	537	91% 9%
1	I	537	90% 9%

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Mol	Chain	Length	Quality of chain
1	K	537	2% 89% 10%
2	B	149	3% 86% 12%
2	D	149	2% 95%
2	F	149	4% 90% 8%
2	H	149	5% 92% 6%
2	J	149	3% 90% 8%
2	L	149	2% 92% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1001	X	-	-	-
4	NAG	A	1002	X	-	-	-
4	NAG	C	1001	X	-	-	-
4	NAG	C	1002	X	-	-	-
4	NAG	E	1001	X	-	-	-
4	NAG	E	1002	X	-	-	-
4	NAG	G	1001	X	-	-	-
4	NAG	G	1002	X	-	-	-
4	NAG	I	1001	X	-	-	-
4	NAG	I	1002	X	-	-	-
4	NAG	K	1001	X	-	-	-
4	NAG	K	1002	X	-	-	-
5	NAG	A	2000	X	-	-	-
5	NAG	C	2000	X	-	-	-
5	NAG	E	2000	X	-	-	-
5	NAG	G	2000	X	-	-	-
5	NAG	I	2000	X	-	-	-
5	NAG	K	2000	X	-	-	-
8	EPE	B	1000	-	-	-	X
8	EPE	D	1000	-	-	-	X
8	EPE	F	1000	-	-	-	X
8	EPE	H	1000	-	-	-	X
8	EPE	J	1000	-	-	-	X
8	EPE	L	1000	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 34132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	C	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	E	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	G	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	I	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			
1	K	537	Total	C	N	O	S	0	0	0
			4315	2763	744	794	14			

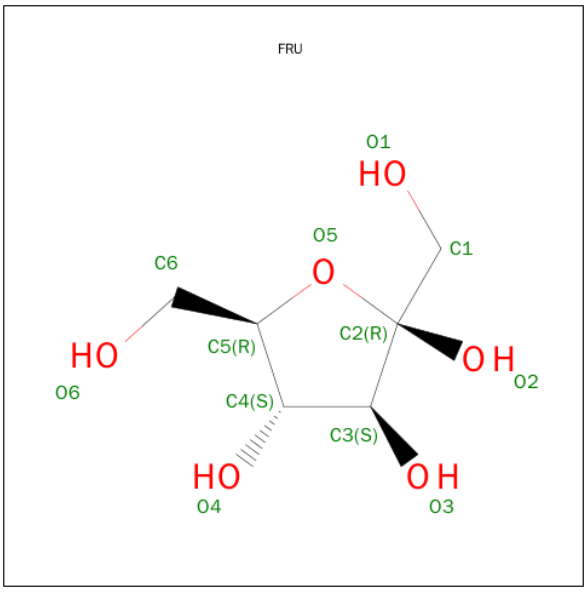
- Molecule 2 is a protein called INVERTASE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	D	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	F	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	H	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	J	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			
2	L	146	Total	C	N	O	S	0	0	0
			1095	690	187	212	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP O49908
D	-1	GLY	-	EXPRESSION TAG	UNP O49908
F	-1	GLY	-	EXPRESSION TAG	UNP O49908
H	-1	GLY	-	EXPRESSION TAG	UNP O49908
J	-1	GLY	-	EXPRESSION TAG	UNP O49908
L	-1	GLY	-	EXPRESSION TAG	UNP O49908

- Molecule 3 is SUGAR (FRUCTOSE) (three-letter code: FRU) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	C	1	Total C O 12 6 6	0	0
3	E	1	Total C O 12 6 6	0	0
3	G	1	Total C O 12 6 6	0	0
3	I	1	Total C O 12 6 6	0	0
3	K	1	Total C O 12 6 6	0	0

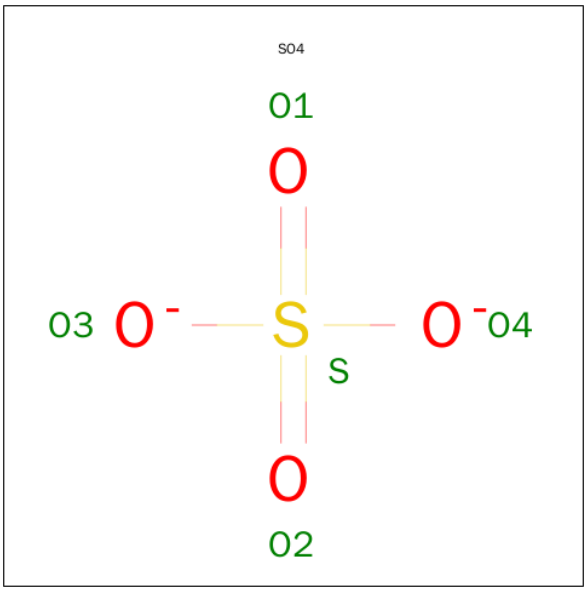
- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	6	Total	C	N	O	0	0
			72	40	2	30		
4	C	6	Total	C	N	O	0	0
			72	40	2	30		
4	E	6	Total	C	N	O	0	0
			72	40	2	30		
4	G	6	Total	C	N	O	0	0
			72	40	2	30		
4	I	6	Total	C	N	O	0	0
			72	40	2	30		
4	K	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

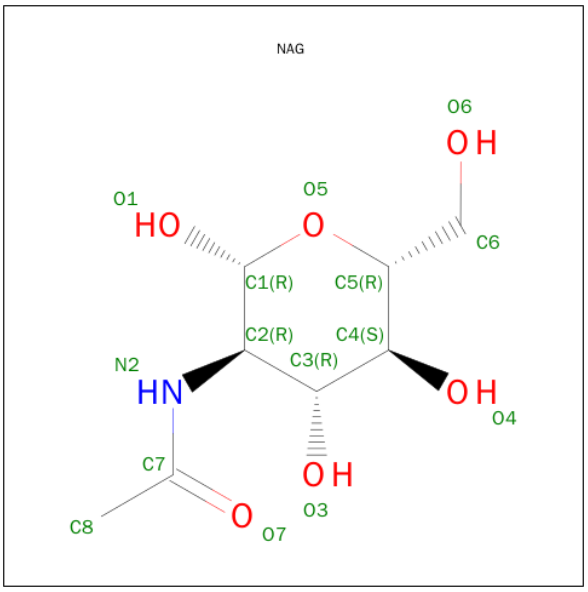
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



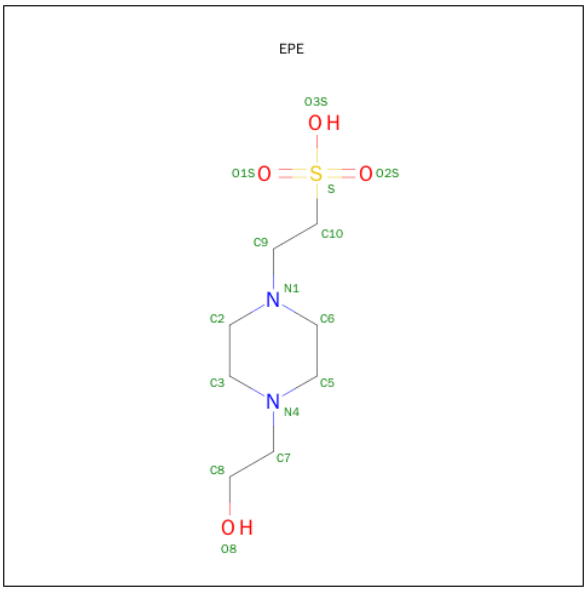
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	I	1	Total O S 5 4 1	0	0
6	K	1	Total O S 5 4 1	0	0

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	G	1	Total C N O 14 8 1 5	0	0
7	I	1	Total C N O 14 8 1 5	0	0
7	K	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	121	Total	O	0	0
			121	121		
9	B	27	Total	O	0	0
			27	27		
9	C	117	Total	O	0	0
			117	117		
9	D	26	Total	O	0	0
			26	26		
9	E	109	Total	O	0	0
			109	109		
9	F	17	Total	O	0	0
			17	17		

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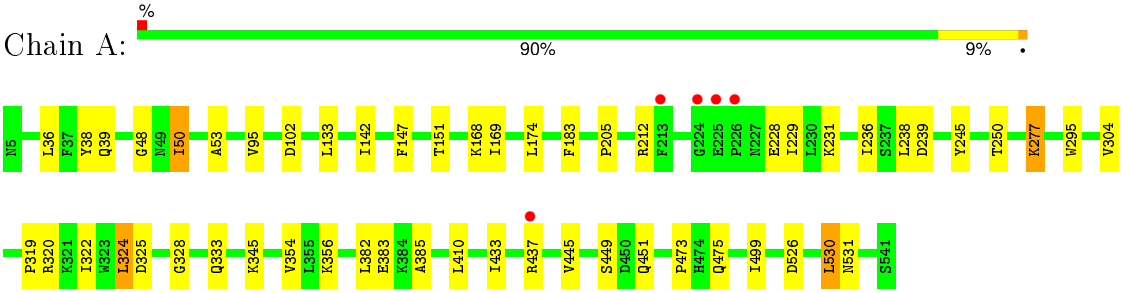
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	99	Total O 99 99	0	0
9	H	20	Total O 20 20	0	0
9	I	106	Total O 106 106	0	0
9	J	29	Total O 29 29	0	0
9	K	98	Total O 98 98	0	0
9	L	22	Total O 22 22	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

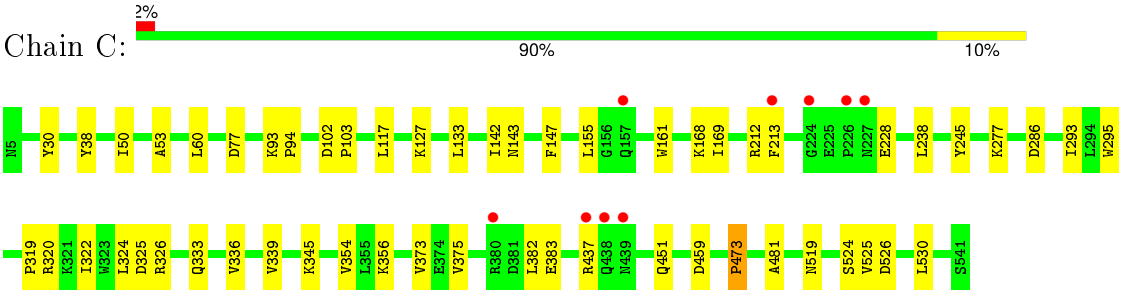
- Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1

Chain A:



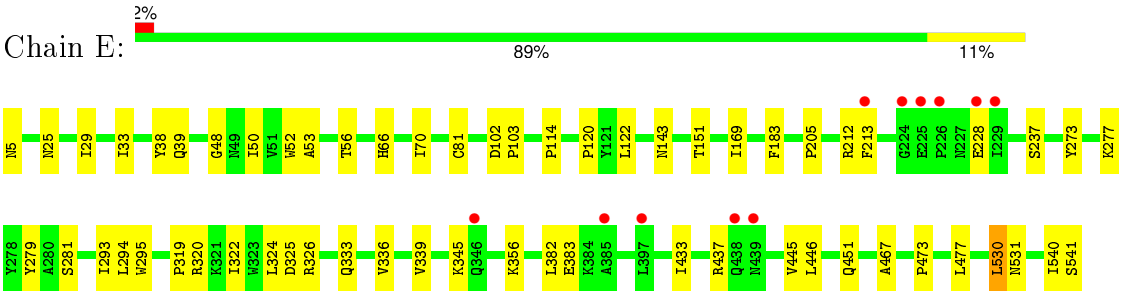
- Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1

Chain C:



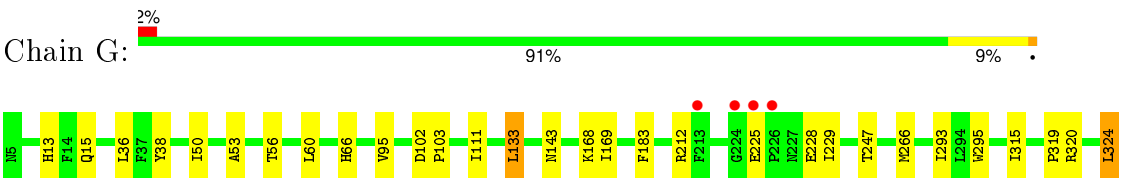
- Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1

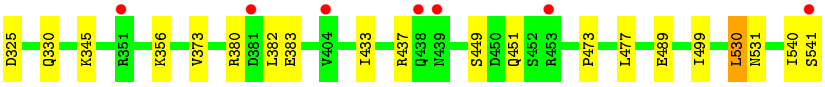
Chain E:



- Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1

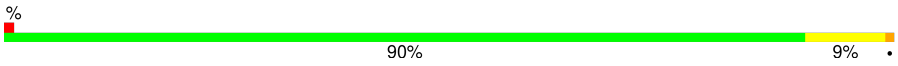
Chain G:

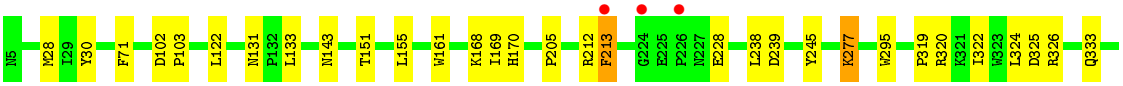


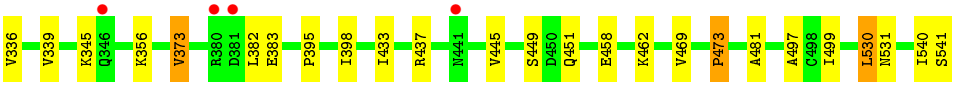


• Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1

Chain I:

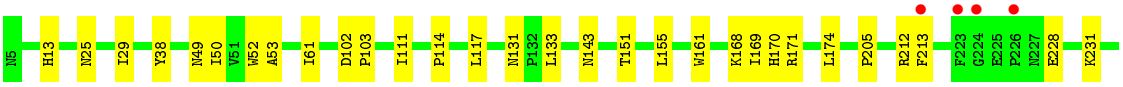


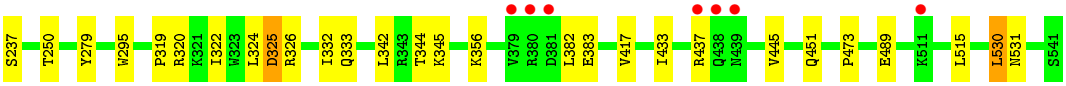




• Molecule 1: BETA-FRUCTOFURANOSIDASE, INSOLUBLE ISOENZYME CWINV1

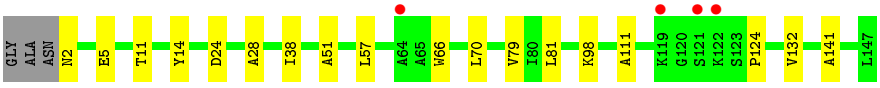
Chain K:





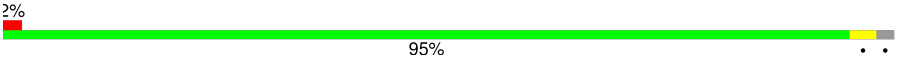
• Molecule 2: INVERTASE INHIBITOR

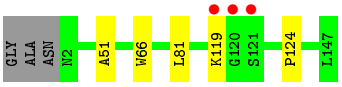
Chain B:



• Molecule 2: INVERTASE INHIBITOR

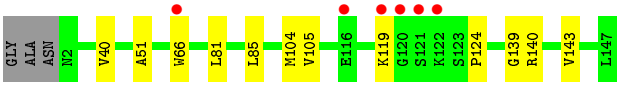
Chain D:





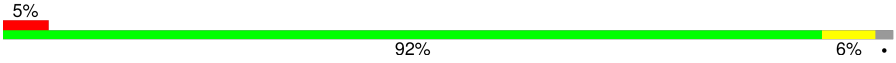
• Molecule 2: INVERTASE INHIBITOR

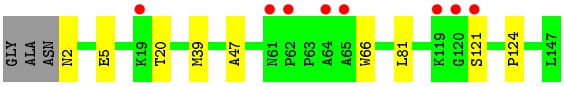
Chain F:



• Molecule 2: INVERTASE INHIBITOR

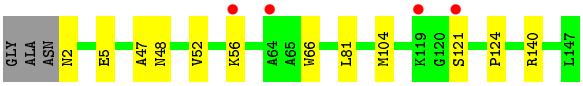
Chain H:





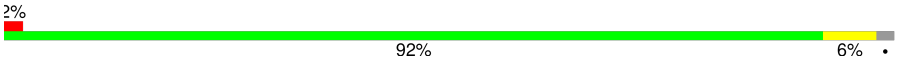
• Molecule 2: INVERTASE INHIBITOR

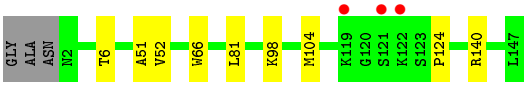
Chain J:



• Molecule 2: INVERTASE INHIBITOR

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	199.98Å 199.98Å 111.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.57 – 2.58 48.58 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.57-2.58) 99.4 (48.58-2.58)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0043	Depositor
R, R_{free}	0.183 , 0.210 0.189 , 0.189	Depositor DCC
R_{free} test set	7782 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 6.1	EDS
Estimated twinning fraction	0.818 for H, K, L 0.182 for -H, H+K, -L 0.057 for -h,-k,l 0.058 for h,-h-k,-l 0.145 for -k,-h,-l	Xtriage
Reported twinning fraction	0.818 for H, K, L 0.182 for -H, H+K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 155624 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	34132	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, SO4, FRU, EPE, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/4442	0.51	0/6034
1	C	0.33	0/4442	0.50	0/6034
1	E	0.32	0/4442	0.50	0/6034
1	G	0.32	0/4442	0.50	0/6034
1	I	0.32	0/4442	0.51	0/6034
1	K	0.32	0/4442	0.50	0/6034
2	B	0.32	0/1112	0.46	0/1506
2	D	0.32	0/1112	0.45	0/1506
2	F	0.33	0/1112	0.45	0/1506
2	H	0.33	0/1112	0.47	0/1506
2	J	0.34	0/1112	0.47	0/1506
2	L	0.33	0/1112	0.46	0/1506
All	All	0.32	0/33324	0.49	0/45240

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	2	0
4	C	2	0
4	E	2	0
4	G	2	0
4	I	2	0
4	K	2	0
5	A	1	0
5	C	1	0
5	E	1	0
5	G	1	0
5	I	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	K	1	0
All	All	18	0

There are no bond length outliers.

There are no bond angle outliers.

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1001	NAG	C1
4	A	1002	NAG	C1
5	A	2000	NAG	C1
4	C	1001	NAG	C1
4	C	1002	NAG	C1
5	C	2000	NAG	C1
4	E	1001	NAG	C1
4	E	1002	NAG	C1
5	E	2000	NAG	C1
4	G	1001	NAG	C1
4	G	1002	NAG	C1
5	G	2000	NAG	C1
4	I	1001	NAG	C1
4	I	1002	NAG	C1
5	I	2000	NAG	C1
4	K	1001	NAG	C1
4	K	1002	NAG	C1
5	K	2000	NAG	C1

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4315	0	4219	28	0
1	C	4315	0	4219	31	0
1	E	4315	0	4219	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4315	0	4219	23	0
1	I	4315	0	4219	31	0
1	K	4315	0	4219	31	0
2	B	1095	0	1118	14	0
2	D	1095	0	1118	4	0
2	F	1095	0	1118	8	0
2	H	1095	0	1118	6	0
2	J	1095	0	1118	8	0
2	L	1095	0	1118	7	0
3	A	12	0	12	1	0
3	C	12	0	12	0	0
3	E	12	0	12	0	0
3	G	12	0	12	0	0
3	I	12	0	12	0	0
3	K	12	0	12	1	0
4	A	72	0	61	2	0
4	C	72	0	61	2	0
4	E	72	0	61	4	0
4	G	72	0	61	0	0
4	I	72	0	61	2	0
4	K	72	0	61	0	0
5	A	28	0	25	0	0
5	C	28	0	25	1	0
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	I	28	0	25	0	0
5	K	28	0	25	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
6	I	5	0	0	1	0
6	K	5	0	0	0	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
7	E	14	0	13	0	0
7	G	14	0	13	0	0
7	I	14	0	13	0	0
7	K	14	0	13	0	0
8	B	15	0	17	3	0
8	D	15	0	17	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	15	0	17	3	0
8	H	15	0	17	2	0
8	J	15	0	17	2	0
8	L	15	0	17	2	0
9	A	121	0	0	0	0
9	B	27	0	0	1	0
9	C	117	0	0	1	0
9	D	26	0	0	1	0
9	E	109	0	0	1	0
9	F	17	0	0	0	0
9	G	99	0	0	0	0
9	H	20	0	0	0	0
9	I	106	0	0	0	0
9	J	29	0	0	0	0
9	K	98	0	0	4	0
9	L	22	0	0	0	0
All	All	34132	0	32790	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:382:LEU:HD21	1:G:473:PRO:HB2	1.72	0.71
1:A:433:ILE:HD12	1:A:445:VAL:HG22	1.72	0.71
2:F:51:ALA:HB1	8:F:1000:EPE:H82	1.74	0.69
1:K:382:LEU:HD21	1:K:473:PRO:HB2	1.75	0.69
1:G:530:LEU:C	1:G:530:LEU:HD12	2.14	0.69
1:K:433:ILE:HD12	1:K:445:VAL:HG22	1.76	0.68
1:C:354:VAL:HG22	1:C:526:ASP:OD1	1.94	0.67
1:E:382:LEU:HD21	1:E:473:PRO:HB2	1.76	0.67
1:C:60:LEU:HD11	1:C:293:ILE:HD13	1.78	0.66
2:B:81:LEU:HD12	8:B:1000:EPE:H32	1.78	0.65
2:B:11:THR:HG22	2:B:141:ALA:HB3	1.79	0.65
1:C:77:ASP:OD2	1:C:127:LYS:NZ	2.29	0.63
1:C:286:ASP:HB2	1:C:293:ILE:HD12	1.81	0.63
1:G:433:ILE:HD11	1:G:477:LEU:HD21	1.79	0.62
1:A:530:LEU:HD12	1:A:530:LEU:C	2.20	0.62
1:E:433:ILE:HD11	1:E:477:LEU:HD21	1.80	0.62
1:I:530:LEU:HD12	1:I:531:ASN:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:213:PHE:CZ	1:I:326:ARG:HG2	2.36	0.60
1:C:373:VAL:HG13	1:C:481:ALA:HB3	1.82	0.60
1:C:382:LEU:HD21	1:C:473:PRO:HB2	1.85	0.59
1:E:48:GLY:O	1:E:50:ILE:HD12	2.04	0.58
5:C:2000:NAG:H83	9:C:4040:HOH:O	2.04	0.58
1:C:213:PHE:CZ	1:C:326:ARG:HG2	2.39	0.57
1:I:382:LEU:HD21	1:I:473:PRO:HB2	1.87	0.57
1:A:385:ALA:HB2	1:A:410:LEU:HD23	1.86	0.57
2:J:81:LEU:HD12	8:J:1000:EPE:H32	1.87	0.57
1:A:277:LYS:HZ3	4:A:1001:NAG:H61	1.70	0.57
1:K:530:LEU:C	1:K:530:LEU:HD12	2.25	0.56
1:G:143:ASN:OD1	1:G:169:ILE:HD13	2.05	0.56
1:I:71:PHE:CE2	2:L:52:VAL:HG21	2.41	0.56
1:I:322:ILE:HG22	1:I:333:GLN:HG2	1.89	0.55
1:K:322:ILE:HG22	1:K:333:GLN:HG2	1.89	0.55
1:K:155:LEU:HD13	1:K:161:TRP:CE2	2.42	0.54
1:E:322:ILE:HG22	1:E:333:GLN:HG2	1.90	0.54
1:E:530:LEU:HD12	1:E:531:ASN:N	2.22	0.54
2:J:47:ALA:HB3	2:J:81:LEU:HD21	1.89	0.54
1:C:213:PHE:CD1	1:E:213:PHE:CE1	2.96	0.53
1:E:433:ILE:HD12	1:E:445:VAL:HG22	1.91	0.53
1:I:238:LEU:HD12	1:I:245:TYR:CE1	2.44	0.53
1:K:417:VAL:HG12	1:K:515:LEU:CD1	2.39	0.53
2:B:81:LEU:HD12	8:B:1000:EPE:C3	2.39	0.53
2:F:81:LEU:HD12	8:F:1000:EPE:H32	1.90	0.53
2:J:81:LEU:HD12	8:J:1000:EPE:C3	2.39	0.53
2:D:81:LEU:HD12	8:D:1000:EPE:H32	1.91	0.52
2:D:119:LYS:NZ	9:D:4023:HOH:O	2.41	0.52
1:A:38:TYR:CZ	1:A:53:ALA:HB3	2.45	0.52
1:C:238:LEU:HD12	1:C:245:TYR:CE1	2.44	0.52
1:C:277:LYS:HZ3	4:C:1001:NAG:H61	1.75	0.52
1:I:155:LEU:HD13	1:I:161:TRP:CE2	2.45	0.51
1:K:171:ARG:NH1	9:K:4042:HOH:O	2.43	0.51
1:E:281:SER:HB2	1:E:294:LEU:HD11	1.93	0.51
2:B:51:ALA:HB1	8:B:1000:EPE:H82	1.93	0.51
1:C:375:VAL:HB	1:C:530:LEU:HD13	1.92	0.51
1:C:322:ILE:HG22	1:C:333:GLN:HG2	1.93	0.51
1:I:71:PHE:CZ	2:L:52:VAL:HG21	2.45	0.51
1:C:213:PHE:HB3	1:E:213:PHE:CD2	2.46	0.51
1:A:36:LEU:HD22	1:A:295:TRP:CH2	2.45	0.51
1:I:277:LYS:NZ	4:I:1001:NAG:H61	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:TRP:CH2	2:F:124:PRO:HG3	2.47	0.50
1:E:273:TYR:CA	1:E:333:GLN:HE22	2.24	0.50
2:F:139:GLY:O	2:F:143:VAL:HG23	2.11	0.50
1:C:38:TYR:CE2	1:C:53:ALA:HB3	2.46	0.50
1:C:213:PHE:CE1	1:E:213:PHE:CE1	3.00	0.49
1:A:295:TRP:CH2	1:A:319:PRO:HG3	2.47	0.49
1:C:93:LYS:HG3	1:C:117:LEU:HD21	1.93	0.49
1:K:143:ASN:OD1	1:K:169:ILE:HD13	2.12	0.49
1:A:277:LYS:NZ	4:A:1001:NAG:H61	2.27	0.49
1:K:530:LEU:HD12	1:K:531:ASN:N	2.26	0.49
1:C:295:TRP:CH2	1:C:319:PRO:HG3	2.47	0.49
1:I:277:LYS:HZ3	4:I:1001:NAG:H61	1.77	0.49
1:A:433:ILE:CD1	1:A:445:VAL:HG22	2.42	0.49
1:E:295:TRP:CH2	1:E:319:PRO:HG3	2.48	0.49
2:B:66:TRP:CH2	2:B:124:PRO:HG3	2.48	0.49
1:E:277:LYS:HZ3	4:E:1001:NAG:H61	1.78	0.49
1:A:151:THR:HG22	1:A:205:PRO:O	2.12	0.49
2:L:81:LEU:HD12	8:L:1000:EPE:H32	1.93	0.49
1:A:229:ILE:HD13	1:G:229:ILE:HD12	1.94	0.49
2:H:81:LEU:HD12	8:H:1000:EPE:H32	1.95	0.48
1:K:295:TRP:CH2	1:K:319:PRO:HG3	2.48	0.48
1:A:324:LEU:HD22	1:A:328:GLY:HA2	1.94	0.48
1:K:61:ILE:CG2	1:K:342:LEU:HD11	2.44	0.48
1:G:95:VAL:HG21	1:G:183:PHE:CE2	2.48	0.48
1:E:336:VAL:O	1:E:339:VAL:HG12	2.13	0.48
1:G:530:LEU:HD12	1:G:531:ASN:N	2.27	0.48
1:I:530:LEU:C	1:I:530:LEU:HD12	2.34	0.48
1:G:324:LEU:HD23	1:G:330:GLN:O	2.14	0.48
1:G:449:SER:HB3	1:G:499:ILE:HG21	1.95	0.48
1:A:382:LEU:HD21	1:A:473:PRO:HB2	1.95	0.48
1:K:213:PHE:CZ	1:K:326:ARG:HG2	2.49	0.48
2:J:66:TRP:CH2	2:J:124:PRO:HG3	2.49	0.48
1:I:295:TRP:CH2	1:I:319:PRO:HG3	2.48	0.48
2:H:20:THR:HG21	2:H:39:MET:SD	2.54	0.47
1:G:247:THR:HG23	1:G:266:MET:HE3	1.96	0.47
1:G:530:LEU:C	1:G:530:LEU:CD1	2.80	0.47
1:I:469:VAL:HG22	1:I:497:ALA:CB	2.44	0.47
2:B:5:GLU:OE1	2:B:14:TYR:OH	2.25	0.47
1:E:114:PRO:HB3	1:E:122:LEU:HD22	1.97	0.47
2:D:51:ALA:HB1	8:D:1000:EPE:H82	1.96	0.47
1:I:469:VAL:HG22	1:I:497:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:ILE:CD1	1:E:445:VAL:HG22	2.45	0.47
1:E:25:ASN:HB3	1:E:52:TRP:CH2	2.50	0.47
1:I:449:SER:HB3	1:I:499:ILE:HG21	1.96	0.47
1:I:143:ASN:OD1	1:I:169:ILE:HD13	2.15	0.46
1:G:36:LEU:HD22	1:G:295:TRP:CH2	2.50	0.46
1:A:48:GLY:H	1:A:50:ILE:HD13	1.80	0.46
1:I:336:VAL:O	1:I:339:VAL:HG12	2.16	0.46
1:E:213:PHE:CZ	1:E:326:ARG:HG2	2.51	0.46
1:I:28:MET:CE	1:I:30:TYR:HB2	2.45	0.46
1:K:25:ASN:HB3	1:K:52:TRP:CH2	2.51	0.46
1:K:102:ASP:HB2	1:K:103:PRO:CD	2.46	0.46
1:I:433:ILE:HD12	1:I:445:VAL:HG22	1.98	0.46
1:E:530:LEU:HD12	1:E:530:LEU:C	2.36	0.46
1:K:111:ILE:HB	1:K:133:LEU:HD22	1.98	0.45
1:E:237:SER:HB3	1:E:279:TYR:CZ	2.51	0.45
1:I:151:THR:HG22	1:I:205:PRO:O	2.16	0.45
2:F:51:ALA:CB	8:F:1000:EPE:H82	2.46	0.45
4:E:1002:NAG:C7	2:F:105:VAL:HG11	2.47	0.45
1:K:13:HIS:NE2	1:K:489:GLU:OE2	2.47	0.45
1:G:38:TYR:CZ	1:G:53:ALA:HB3	2.52	0.45
1:G:295:TRP:CH2	1:G:319:PRO:HG3	2.51	0.45
1:E:33:ILE:HD12	1:E:120:PRO:HB2	1.99	0.45
1:C:373:VAL:CG1	1:C:481:ALA:HB3	2.47	0.45
2:F:40:VAL:HG13	2:F:85:LEU:HD22	1.99	0.45
2:B:11:THR:HG22	2:B:141:ALA:CB	2.46	0.45
1:C:213:PHE:HB3	1:E:213:PHE:CE2	2.51	0.45
1:E:102:ASP:HB2	1:E:103:PRO:CD	2.48	0.44
1:A:449:SER:HB3	1:A:499:ILE:HG21	1.99	0.44
1:C:155:LEU:HD13	1:C:161:TRP:CE2	2.52	0.44
1:G:15:GLN:HB3	1:G:315:ILE:HG22	2.00	0.44
1:G:102:ASP:HB2	1:G:103:PRO:CD	2.48	0.44
2:B:2:ASN:HB2	2:B:5:GLU:HB2	1.99	0.44
2:J:2:ASN:HB2	2:J:5:GLU:HB3	2.00	0.44
2:H:2:ASN:HB2	2:H:5:GLU:HB2	2.00	0.43
1:I:395:PRO:HA	1:I:398:ILE:HD12	2.01	0.43
1:A:238:LEU:HD12	1:A:245:TYR:CE1	2.53	0.43
1:K:344:THR:HG21	9:K:4065:HOH:O	2.18	0.43
1:E:70:ILE:HG22	1:E:81:CYS:SG	2.58	0.43
2:J:48:ASN:O	2:J:52:VAL:HG23	2.18	0.43
1:I:143:ASN:ND2	6:I:2002:SO4:O1	2.50	0.43
1:K:151:THR:HG22	1:K:205:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:LEU:HD12	1:E:467:ALA:O	2.17	0.43
1:C:143:ASN:OD1	1:C:169:ILE:HD13	2.18	0.43
2:L:51:ALA:HB1	8:L:1000:EPE:H82	2.01	0.43
3:A:1000:FRU:O2	2:B:98:LYS:NZ	2.52	0.43
2:J:47:ALA:CB	2:J:81:LEU:HD21	2.48	0.43
1:C:60:LEU:CD1	1:C:293:ILE:HD13	2.46	0.43
1:C:38:TYR:CZ	1:C:53:ALA:HB3	2.54	0.43
2:B:24:ASP:HB3	2:B:38:ILE:HD13	2.00	0.43
1:I:373:VAL:HG23	1:I:530:LEU:CD1	2.48	0.43
1:A:236:ILE:HD12	1:A:238:LEU:HD21	2.01	0.43
1:K:325:ASP:CB	1:K:332:ILE:HD11	2.48	0.43
1:A:322:ILE:HG22	1:A:333:GLN:HG2	2.00	0.43
1:K:237:SER:HB3	1:K:279:TYR:CZ	2.54	0.43
1:A:530:LEU:HD12	1:A:531:ASN:N	2.32	0.43
1:K:38:TYR:CZ	1:K:53:ALA:HB3	2.53	0.43
1:K:169:ILE:HG12	1:K:174:LEU:HD11	2.00	0.42
1:E:143:ASN:OD1	1:E:169:ILE:HD13	2.19	0.42
2:H:66:TRP:CH2	2:H:124:PRO:HG3	2.54	0.42
1:E:151:THR:HG22	1:E:205:PRO:O	2.18	0.42
1:G:540:ILE:O	1:G:541:SER:C	2.57	0.42
1:A:385:ALA:CB	1:A:410:LEU:HD23	2.48	0.42
2:H:47:ALA:HB3	2:H:81:LEU:HD21	2.01	0.42
1:A:39:GLN:OE1	1:A:50:ILE:HG21	2.19	0.42
1:K:231:LYS:NZ	1:K:250:THR:HG23	2.34	0.42
2:B:28:ALA:HB3	9:B:4008:HOH:O	2.18	0.42
1:I:131:ASN:OD1	1:I:133:LEU:HD13	2.19	0.42
1:K:131:ASN:OD1	1:K:133:LEU:HD13	2.19	0.42
1:G:60:LEU:CD1	1:G:293:ILE:HD13	2.50	0.42
2:D:66:TRP:CH2	2:D:124:PRO:HG3	2.54	0.42
1:K:231:LYS:HZ1	1:K:250:THR:HG23	1.85	0.42
1:G:13:HIS:NE2	1:G:489:GLU:OE2	2.48	0.42
1:K:114:PRO:HB2	1:K:117:LEU:HD23	2.01	0.42
1:C:373:VAL:HG23	1:C:530:LEU:HD11	2.02	0.42
1:K:29:ILE:HG23	9:K:4055:HOH:O	2.20	0.42
1:C:356:LYS:HA	1:C:524:SER:HB3	2.00	0.42
1:E:5:ASN:N	9:E:4002:HOH:O	2.52	0.42
1:C:277:LYS:NZ	4:C:1001:NAG:H61	2.35	0.42
1:K:170:HIS:H	5:K:2000:NAG:H83	1.84	0.42
1:I:169:ILE:HG22	1:I:170:HIS:CD2	2.55	0.42
1:E:29:ILE:HD12	1:E:33:ILE:O	2.20	0.42
1:E:273:TYR:O	1:E:333:GLN:NE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ILE:HD13	1:E:336:VAL:HG11	2.02	0.41
1:I:30:TYR:CD2	1:I:122:LEU:HD11	2.54	0.41
2:F:104:MET:HB3	2:F:140:ARG:HG3	2.02	0.41
1:C:142:ILE:HG21	1:C:147:PHE:CD1	2.55	0.41
1:K:169:ILE:HG22	1:K:170:HIS:CD2	2.55	0.41
1:G:111:ILE:HB	1:G:133:LEU:CD2	2.50	0.41
1:C:102:ASP:HB2	1:C:103:PRO:CD	2.50	0.41
2:H:81:LEU:HD12	8:H:1000:EPE:C3	2.50	0.41
1:A:142:ILE:HG21	1:A:147:PHE:CD1	2.56	0.41
1:G:449:SER:CB	1:G:499:ILE:HG21	2.50	0.41
2:B:111:ALA:HB2	2:B:132:VAL:HG12	2.01	0.41
2:J:104:MET:HB3	2:J:140:ARG:HG3	2.02	0.41
1:K:61:ILE:HG21	1:K:342:LEU:HD11	2.02	0.41
1:A:304:VAL:HG13	2:B:79:VAL:HG11	2.02	0.41
1:A:354:VAL:HG22	1:A:526:ASP:OD1	2.20	0.41
1:A:95:VAL:HG21	1:A:183:PHE:CE2	2.55	0.41
1:E:56:THR:HG23	1:E:66:HIS:CD2	2.56	0.41
1:G:373:VAL:HG23	1:G:530:LEU:CD1	2.51	0.41
1:A:38:TYR:CE2	1:A:53:ALA:HB3	2.56	0.41
1:I:540:ILE:O	1:I:541:SER:C	2.57	0.41
1:E:273:TYR:C	1:E:333:GLN:HE22	2.24	0.41
1:K:326:ARG:NH2	9:K:4060:HOH:O	2.53	0.41
2:B:57:LEU:HB2	2:B:70:LEU:HD21	2.03	0.41
1:E:39:GLN:OE1	1:E:50:ILE:HG21	2.20	0.41
3:K:1000:FRU:O2	2:L:98:LYS:NZ	2.53	0.41
1:A:231:LYS:HZ1	1:A:250:THR:HG23	1.86	0.41
1:E:277:LYS:HZ3	4:E:1001:NAG:C6	2.33	0.40
1:C:519:ASN:ND2	1:C:525:VAL:HG22	2.36	0.40
1:C:336:VAL:O	1:C:339:VAL:HG12	2.20	0.40
1:G:56:THR:HG23	1:G:66:HIS:CD2	2.57	0.40
2:L:104:MET:HB3	2:L:140:ARG:HG3	2.02	0.40
1:E:540:ILE:O	1:E:541:SER:C	2.58	0.40
1:E:38:TYR:CZ	1:E:53:ALA:HB3	2.56	0.40
1:A:169:ILE:HG12	1:A:174:LEU:HD11	2.03	0.40
1:C:30:TYR:CE1	1:C:94:PRO:HD3	2.57	0.40
4:E:1003:BMA:H62	4:E:1005:BMA:C6	2.51	0.40
1:I:373:VAL:HG13	1:I:481:ALA:HB3	2.04	0.40
1:I:373:VAL:HG23	1:I:530:LEU:HD11	2.03	0.40
2:L:66:TRP:CH2	2:L:124:PRO:HG3	2.57	0.40
1:I:458:GLU:HA	1:I:462:LYS:NZ	2.36	0.40
1:I:102:ASP:HB2	1:I:103:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	535/537 (100%)	508 (95%)	27 (5%)	0	100	100
1	C	535/537 (100%)	511 (96%)	24 (4%)	0	100	100
1	E	535/537 (100%)	509 (95%)	26 (5%)	0	100	100
1	G	535/537 (100%)	513 (96%)	22 (4%)	0	100	100
1	I	535/537 (100%)	511 (96%)	24 (4%)	0	100	100
1	K	535/537 (100%)	511 (96%)	24 (4%)	0	100	100
2	B	144/149 (97%)	136 (94%)	8 (6%)	0	100	100
2	D	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
2	F	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
2	H	144/149 (97%)	137 (95%)	6 (4%)	1 (1%)	26	49
2	J	144/149 (97%)	137 (95%)	6 (4%)	1 (1%)	26	49
2	L	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
All	All	4074/4116 (99%)	3887 (95%)	185 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	121	SER
2	J	121	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	473/473 (100%)	455 (96%)	18 (4%)	40 67
1	C	473/473 (100%)	459 (97%)	14 (3%)	48 75
1	E	473/473 (100%)	461 (98%)	12 (2%)	55 79
1	G	473/473 (100%)	457 (97%)	16 (3%)	44 71
1	I	473/473 (100%)	456 (96%)	17 (4%)	42 69
1	K	473/473 (100%)	459 (97%)	14 (3%)	48 75
2	B	120/121 (99%)	120 (100%)	0	100 100
2	D	120/121 (99%)	120 (100%)	0	100 100
2	F	120/121 (99%)	119 (99%)	1 (1%)	86 95
2	H	120/121 (99%)	120 (100%)	0	100 100
2	J	120/121 (99%)	119 (99%)	1 (1%)	86 95
2	L	120/121 (99%)	119 (99%)	1 (1%)	86 95
All	All	3558/3564 (100%)	3464 (97%)	94 (3%)	54 78

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	102	ASP
1	A	133	LEU
1	A	168	LYS
1	A	212	ARG
1	A	228	GLU
1	A	239	ASP
1	A	277	LYS
1	A	320	ARG
1	A	324	LEU
1	A	325	ASP
1	A	345	LYS
1	A	356	LYS
1	A	383	GLU
1	A	437	ARG
1	A	451	GLN
1	A	475	GLN
1	A	530	LEU
1	C	50	ILE

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Mol	Chain	Res	Type
1	C	133	LEU
1	C	168	LYS
1	C	212	ARG
1	C	228	GLU
1	C	320	ARG
1	C	324	LEU
1	C	325	ASP
1	C	345	LYS
1	C	383	GLU
1	C	437	ARG
1	C	451	GLN
1	C	459	ASP
1	C	473	PRO
1	E	183	PHE
1	E	212	ARG
1	E	228	GLU
1	E	320	ARG
1	E	324	LEU
1	E	325	ASP
1	E	345	LYS
1	E	356	LYS
1	E	383	GLU
1	E	437	ARG
1	E	451	GLN
1	E	530	LEU
2	F	119	LYS
1	G	50	ILE
1	G	133	LEU
1	G	168	LYS
1	G	212	ARG
1	G	225	GLU
1	G	228	GLU
1	G	320	ARG
1	G	324	LEU
1	G	325	ASP
1	G	345	LYS
1	G	356	LYS
1	G	380	ARG
1	G	383	GLU
1	G	437	ARG
1	G	451	GLN
1	G	530	LEU

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Mol	Chain	Res	Type
1	I	168	LYS
1	I	212	ARG
1	I	213	PHE
1	I	228	GLU
1	I	239	ASP
1	I	277	LYS
1	I	320	ARG
1	I	324	LEU
1	I	325	ASP
1	I	345	LYS
1	I	356	LYS
1	I	373	VAL
1	I	383	GLU
1	I	437	ARG
1	I	451	GLN
1	I	473	PRO
1	I	530	LEU
2	J	56	LYS
1	K	49	ASN
1	K	50	ILE
1	K	168	LYS
1	K	212	ARG
1	K	228	GLU
1	K	320	ARG
1	K	324	LEU
1	K	325	ASP
1	K	345	LYS
1	K	356	LYS
1	K	383	GLU
1	K	437	ARG
1	K	451	GLN
1	K	530	LEU
2	L	6	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	2	ASN
2	B	61	ASN
1	C	262	ASN
1	C	333	GLN
1	C	439	ASN

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Mol	Chain	Res	Type
1	C	475	GLN
2	D	10	ASN
2	D	61	ASN
1	E	333	GLN
1	E	475	GLN
2	F	10	ASN
1	G	170	HIS
1	G	243	HIS
1	G	262	ASN
1	G	451	GLN
2	H	2	ASN
2	J	2	ASN
1	K	170	HIS
1	K	333	GLN
2	L	61	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

48 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1001	1,4	14,14,15	0.53	0	15,19,21	1.29	1 (6%)
4	NAG	A	1002	4	14,14,15	0.57	0	15,19,21	1.23	1 (6%)
4	BMA	A	1003	4	11,11,12	0.57	0	14,15,17	2.16	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	A	1004	4	11,11,12	0.64	0	14,15,17	0.66	0
4	BMA	A	1005	4	11,11,12	0.49	0	14,15,17	2.59	2 (14%)
4	MAN	A	1006	4	11,11,12	0.46	0	14,15,17	0.86	0
5	NAG	A	2000	1,5	14,14,15	0.47	0	15,19,21	1.62	4 (26%)
5	NAG	A	2001	5	14,14,15	0.47	0	15,19,21	0.89	0
4	NAG	C	1001	1,4	14,14,15	0.49	0	15,19,21	1.18	1 (6%)
4	NAG	C	1002	4	14,14,15	0.58	0	15,19,21	1.37	1 (6%)
4	BMA	C	1003	4	11,11,12	0.43	0	14,15,17	2.25	4 (28%)
4	MAN	C	1004	4	11,11,12	0.61	0	14,15,17	0.82	1 (7%)
4	BMA	C	1005	4	11,11,12	0.46	0	14,15,17	2.66	2 (14%)
4	MAN	C	1006	4	11,11,12	0.56	0	14,15,17	0.80	0
5	NAG	C	2000	1,5	14,14,15	0.58	0	15,19,21	1.73	5 (33%)
5	NAG	C	2001	5	14,14,15	0.51	0	15,19,21	0.75	0
4	NAG	E	1001	1,4	14,14,15	0.47	0	15,19,21	1.30	1 (6%)
4	NAG	E	1002	4	14,14,15	0.56	0	15,19,21	1.46	1 (6%)
4	BMA	E	1003	4	11,11,12	0.55	0	14,15,17	1.95	2 (14%)
4	MAN	E	1004	4	11,11,12	0.56	0	14,15,17	0.74	1 (7%)
4	BMA	E	1005	4	11,11,12	0.45	0	14,15,17	2.55	2 (14%)
4	MAN	E	1006	4	11,11,12	0.51	0	14,15,17	0.78	0
5	NAG	E	2000	1,5	14,14,15	0.52	0	15,19,21	1.50	3 (20%)
5	NAG	E	2001	5	14,14,15	0.49	0	15,19,21	0.87	0
4	NAG	G	1001	1,4	14,14,15	0.58	0	15,19,21	1.34	2 (13%)
4	NAG	G	1002	4	14,14,15	0.58	0	15,19,21	1.01	1 (6%)
4	BMA	G	1003	4	11,11,12	0.59	0	14,15,17	2.34	4 (28%)
4	MAN	G	1004	4	11,11,12	0.63	0	14,15,17	0.47	0
4	BMA	G	1005	4	11,11,12	0.51	0	14,15,17	2.50	2 (14%)
4	MAN	G	1006	4	11,11,12	0.59	0	14,15,17	0.98	1 (7%)
5	NAG	G	2000	1,5	14,14,15	0.56	0	15,19,21	1.28	2 (13%)
5	NAG	G	2001	5	14,14,15	0.50	0	15,19,21	0.96	1 (6%)
4	NAG	I	1001	1,4	14,14,15	0.55	0	15,19,21	1.29	1 (6%)
4	NAG	I	1002	4	14,14,15	0.62	0	15,19,21	0.88	1 (6%)
4	BMA	I	1003	4	11,11,12	0.61	0	14,15,17	2.28	2 (14%)
4	MAN	I	1004	4	11,11,12	0.55	0	14,15,17	1.12	1 (7%)
4	BMA	I	1005	4	11,11,12	0.47	0	14,15,17	2.52	2 (14%)
4	MAN	I	1006	4	11,11,12	0.66	0	14,15,17	1.31	2 (14%)
5	NAG	I	2000	1,5	14,14,15	0.49	0	15,19,21	1.69	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	I	2001	5	14,14,15	0.51	0	15,19,21	0.65	0
4	NAG	K	1001	1,4	14,14,15	0.52	0	15,19,21	1.36	1 (6%)
4	NAG	K	1002	4	14,14,15	0.59	0	15,19,21	1.44	1 (6%)
4	BMA	K	1003	4	11,11,12	0.52	0	14,15,17	2.54	2 (14%)
4	MAN	K	1004	4	11,11,12	0.61	0	14,15,17	0.73	0
4	BMA	K	1005	4	11,11,12	0.45	0	14,15,17	2.65	2 (14%)
4	MAN	K	1006	4	11,11,12	0.54	0	14,15,17	0.82	0
5	NAG	K	2000	1,5	14,14,15	0.55	0	15,19,21	1.34	2 (13%)
5	NAG	K	2001	5	14,14,15	0.50	0	15,19,21	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1002	4	1/1/5/7	0/6/23/26	0/1/1/1
4	BMA	A	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1004	4	-	0/2/19/22	0/1/1/1
4	BMA	A	1005	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1006	4	-	0/2/19/22	0/1/1/1
5	NAG	A	2000	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	2001	5	-	0/6/23/26	0/1/1/1
4	NAG	C	1001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	1002	4	1/1/5/7	0/6/23/26	0/1/1/1
4	BMA	C	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	C	1004	4	-	0/2/19/22	0/1/1/1
4	BMA	C	1005	4	-	0/2/19/22	0/1/1/1
4	MAN	C	1006	4	-	0/2/19/22	0/1/1/1
5	NAG	C	2000	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	C	2001	5	-	0/6/23/26	0/1/1/1
4	NAG	E	1001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	E	1002	4	1/1/5/7	0/6/23/26	0/1/1/1
4	BMA	E	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	E	1004	4	-	0/2/19/22	0/1/1/1
4	BMA	E	1005	4	-	0/2/19/22	0/1/1/1
4	MAN	E	1006	4	-	0/2/19/22	0/1/1/1
5	NAG	E	2000	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	2001	5	-	0/6/23/26	0/1/1/1
4	NAG	G	1001	1,4	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1002	4	1/1/5/7	0/6/23/26	0/1/1/1
4	BMA	G	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	G	1004	4	-	0/2/19/22	0/1/1/1
4	BMA	G	1005	4	-	0/2/19/22	0/1/1/1
4	MAN	G	1006	4	-	0/2/19/22	0/1/1/1
5	NAG	G	2000	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	2001	5	-	0/6/23/26	0/1/1/1
4	NAG	I	1001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	I	1002	4	1/1/5/7	0/6/23/26	0/1/1/1
4	BMA	I	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	I	1004	4	-	0/2/19/22	0/1/1/1
4	BMA	I	1005	4	-	0/2/19/22	0/1/1/1
4	MAN	I	1006	4	-	0/2/19/22	0/1/1/1
5	NAG	I	2000	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	I	2001	5	-	0/6/23/26	0/1/1/1
4	NAG	K	1001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	K	1002	4	1/1/5/7	0/6/23/26	0/1/1/1
4	BMA	K	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	K	1004	4	-	0/2/19/22	0/1/1/1
4	BMA	K	1005	4	-	0/2/19/22	0/1/1/1
4	MAN	K	1006	4	-	0/2/19/22	0/1/1/1
5	NAG	K	2000	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	K	2001	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1003	BMA	O3-C3-C4	-2.69	104.27	110.34
4	G	1006	MAN	O5-C1-C2	-2.50	106.81	110.86
4	C	1003	BMA	C6-C5-C4	-2.33	107.26	113.02
4	A	1003	BMA	O3-C3-C4	-2.18	105.43	110.34
5	C	2000	NAG	O7-C7-C8	-2.17	118.08	122.06
4	G	1003	BMA	O3-C3-C4	-2.15	105.50	110.34
5	I	2000	NAG	O7-C7-C8	-2.02	118.36	122.06
4	G	1003	BMA	C6-C5-C4	-2.01	108.05	113.02
5	G	2001	NAG	C1-O5-C5	2.01	114.79	112.25
5	E	2000	NAG	C3-C2-N2	2.01	115.38	110.56
4	C	1004	MAN	C1-O5-C5	2.07	114.88	112.25
4	I	1002	NAG	C1-O5-C5	2.11	114.93	112.25
5	C	2000	NAG	O7-C7-N2	2.13	126.20	121.86
5	A	2000	NAG	O7-C7-N2	2.18	126.30	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1004	MAN	C1-O5-C5	2.19	115.03	112.25
5	K	2000	NAG	C3-C2-N2	2.20	115.84	110.56
4	I	1006	MAN	C3-C4-C5	2.21	114.05	110.20
5	G	2000	NAG	C2-N2-C7	2.24	125.92	123.04
4	A	1003	BMA	C1-C2-C3	2.31	112.27	109.54
5	A	2000	NAG	C1-O5-C5	2.31	115.18	112.25
4	G	1001	NAG	O5-C5-C6	2.33	112.39	107.35
4	G	1002	NAG	C1-O5-C5	2.44	115.34	112.25
5	G	2000	NAG	C1-O5-C5	2.48	115.40	112.25
5	K	2000	NAG	C2-N2-C7	2.51	126.26	123.04
5	C	2000	NAG	C1-O5-C5	2.62	115.58	112.25
4	I	1005	BMA	C3-C4-C5	2.64	114.79	110.20
5	E	2000	NAG	C1-O5-C5	2.64	115.59	112.25
4	K	1003	BMA	C3-C4-C5	2.68	114.86	110.20
5	C	2000	NAG	C3-C2-N2	2.73	117.09	110.56
5	E	2000	NAG	C2-N2-C7	2.74	126.56	123.04
4	K	1005	BMA	C3-C4-C5	2.76	115.02	110.20
5	A	2000	NAG	C3-C2-N2	2.83	117.34	110.56
4	I	1006	MAN	C1-C2-C3	2.91	112.98	109.54
4	I	1001	NAG	C1-O5-C5	2.92	115.95	112.25
4	G	1003	BMA	C3-C4-C5	2.94	115.31	110.20
4	C	1005	BMA	C3-C4-C5	3.00	115.43	110.20
4	A	1005	BMA	C3-C4-C5	3.10	115.59	110.20
4	I	1004	MAN	C1-O5-C5	3.10	116.18	112.25
4	E	1005	BMA	C3-C4-C5	3.15	115.69	110.20
4	G	1005	BMA	C3-C4-C5	3.18	115.73	110.20
4	C	1001	NAG	C1-O5-C5	3.19	116.30	112.25
5	I	2000	NAG	C3-C2-N2	3.20	118.21	110.56
4	G	1001	NAG	C1-O5-C5	3.25	116.37	112.25
4	E	1001	NAG	C1-O5-C5	3.39	116.55	112.25
4	A	1001	NAG	C1-O5-C5	3.57	116.78	112.25
4	E	1003	BMA	C3-C4-C5	3.62	116.51	110.20
4	I	1003	BMA	C3-C4-C5	3.66	116.58	110.20
4	C	1003	BMA	C3-C4-C5	3.70	116.65	110.20
5	C	2000	NAG	C2-N2-C7	3.74	127.84	123.04
4	K	1001	NAG	C1-O5-C5	3.76	117.02	112.25
4	A	1003	BMA	C3-C4-C5	3.79	116.81	110.20
4	A	1002	NAG	C1-O5-C5	3.90	117.19	112.25
5	A	2000	NAG	C2-N2-C7	4.08	128.28	123.04
5	I	2000	NAG	C2-N2-C7	4.22	128.46	123.04
4	K	1002	NAG	C1-O5-C5	4.57	118.05	112.25
4	C	1002	NAG	C1-O5-C5	4.59	118.07	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1002	NAG	C1-O5-C5	4.79	118.33	112.25
4	E	1003	BMA	C1-O5-C5	5.26	118.93	112.25
4	A	1003	BMA	C1-O5-C5	5.87	119.69	112.25
4	C	1003	BMA	C1-O5-C5	6.16	120.06	112.25
4	I	1003	BMA	C1-O5-C5	7.01	121.14	112.25
4	G	1003	BMA	C1-O5-C5	7.19	121.37	112.25
4	G	1005	BMA	C1-O5-C5	8.27	122.75	112.25
4	K	1003	BMA	C1-O5-C5	8.44	122.96	112.25
4	I	1005	BMA	C1-O5-C5	8.71	123.31	112.25
4	A	1005	BMA	C1-O5-C5	8.74	123.34	112.25
4	E	1005	BMA	C1-O5-C5	8.82	123.44	112.25
4	C	1005	BMA	C1-O5-C5	9.10	123.80	112.25
4	K	1005	BMA	C1-O5-C5	9.23	123.97	112.25

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	2000	NAG	C1
4	K	1002	NAG	C1
4	E	1001	NAG	C1
5	G	2000	NAG	C1
5	K	2000	NAG	C1
5	E	2000	NAG	C1
4	E	1002	NAG	C1
4	A	1001	NAG	C1
4	C	1001	NAG	C1
4	A	1002	NAG	C1
4	I	1001	NAG	C1
4	K	1001	NAG	C1
4	I	1002	NAG	C1
4	G	1001	NAG	C1
4	C	1002	NAG	C1
5	A	2000	NAG	C1
4	G	1002	NAG	C1
5	I	2000	NAG	C1

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	NAG	2	0
4	C	1001	NAG	2	0
5	C	2000	NAG	1	0
4	E	1001	NAG	2	0
4	E	1002	NAG	1	0
4	E	1003	BMA	1	0
4	E	1005	BMA	1	0
4	I	1001	NAG	2	0
5	K	2000	NAG	1	0

5.6 Ligand geometry (i)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FRU	A	1000	-	11,12,12	0.70	0	10,18,18	0.45	0
6	SO4	A	2002	-	4,4,4	0.12	0	6,6,6	0.15	0
7	NAG	A	3000	1	14,14,15	0.49	0	15,19,21	0.90	1 (6%)
8	EPE	B	1000	-	14,15,15	0.45	0	18,20,20	1.33	2 (11%)
6	SO4	B	1001	-	4,4,4	0.17	0	6,6,6	0.10	0
3	FRU	C	1000	-	11,12,12	0.54	0	10,18,18	0.53	0
6	SO4	C	2002	-	4,4,4	0.16	0	6,6,6	0.22	0
7	NAG	C	3000	1	14,14,15	0.43	0	15,19,21	0.78	0
8	EPE	D	1000	-	14,15,15	0.44	0	18,20,20	1.34	2 (11%)
3	FRU	E	1000	-	11,12,12	0.59	0	10,18,18	0.54	0
6	SO4	E	2002	-	4,4,4	0.14	0	6,6,6	0.19	0
7	NAG	E	3000	1	14,14,15	0.43	0	15,19,21	0.76	0
8	EPE	F	1000	-	14,15,15	0.45	0	18,20,20	1.22	2 (11%)
3	FRU	G	1000	-	11,12,12	0.64	0	10,18,18	0.35	0
6	SO4	G	2002	-	4,4,4	0.13	0	6,6,6	0.20	0
7	NAG	G	3000	1	14,14,15	0.42	0	15,19,21	1.06	1 (6%)
8	EPE	H	1000	-	14,15,15	0.43	0	18,20,20	1.32	2 (11%)
3	FRU	I	1000	-	11,12,12	0.58	0	10,18,18	0.55	0
6	SO4	I	2002	-	4,4,4	0.15	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	I	3000	1	14,14,15	0.41	0	15,19,21	0.80	0
8	EPE	J	1000	-	14,15,15	0.44	0	18,20,20	1.21	1 (5%)
3	FRU	K	1000	-	11,12,12	0.68	0	10,18,18	0.56	0
6	SO4	K	2002	-	4,4,4	0.14	0	6,6,6	0.10	0
7	NAG	K	3000	1	14,14,15	0.43	0	15,19,21	0.95	1 (6%)
8	EPE	L	1000	-	14,15,15	0.40	0	18,20,20	1.29	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRU	A	1000	-	-	0/5/24/24	0/1/1/1
6	SO4	A	2002	-	-	0/0/0/0	0/0/0/0
7	NAG	A	3000	1	-	0/6/23/26	0/1/1/1
8	EPE	B	1000	-	-	0/9/19/19	0/1/1/1
6	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
3	FRU	C	1000	-	-	0/5/24/24	0/1/1/1
6	SO4	C	2002	-	-	0/0/0/0	0/0/0/0
7	NAG	C	3000	1	-	0/6/23/26	0/1/1/1
8	EPE	D	1000	-	-	0/9/19/19	0/1/1/1
3	FRU	E	1000	-	-	0/5/24/24	0/1/1/1
6	SO4	E	2002	-	-	0/0/0/0	0/0/0/0
7	NAG	E	3000	1	-	0/6/23/26	0/1/1/1
8	EPE	F	1000	-	-	0/9/19/19	0/1/1/1
3	FRU	G	1000	-	-	0/5/24/24	0/1/1/1
6	SO4	G	2002	-	-	0/0/0/0	0/0/0/0
7	NAG	G	3000	1	-	0/6/23/26	0/1/1/1
8	EPE	H	1000	-	-	0/9/19/19	0/1/1/1
3	FRU	I	1000	-	-	0/5/24/24	0/1/1/1
6	SO4	I	2002	-	-	0/0/0/0	0/0/0/0
7	NAG	I	3000	1	-	0/6/23/26	0/1/1/1
8	EPE	J	1000	-	-	0/9/19/19	0/1/1/1
3	FRU	K	1000	-	-	0/5/24/24	0/1/1/1
6	SO4	K	2002	-	-	0/0/0/0	0/0/0/0
7	NAG	K	3000	1	-	0/6/23/26	0/1/1/1
8	EPE	L	1000	-	-	0/9/19/19	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	1000	EPE	C2-C3-N4	2.09	114.36	110.63
7	K	3000	NAG	C1-O5-C5	2.12	114.93	112.25
8	L	1000	EPE	O1S-S-C10	2.15	108.74	106.91
8	D	1000	EPE	O2S-S-C10	2.21	108.79	106.91
7	A	3000	NAG	C1-O5-C5	2.49	115.41	112.25
8	F	1000	EPE	O1S-S-C10	2.57	109.10	106.91
8	H	1000	EPE	O2S-S-C10	3.01	109.47	106.91
8	H	1000	EPE	O1S-S-C10	3.02	109.48	106.91
8	F	1000	EPE	O2S-S-C10	3.06	109.52	106.91
8	B	1000	EPE	O1S-S-C10	3.07	109.52	106.91
8	B	1000	EPE	O2S-S-C10	3.10	109.55	106.91
7	G	3000	NAG	C1-O5-C5	3.15	116.24	112.25
8	J	1000	EPE	O1S-S-C10	3.31	109.73	106.91
8	L	1000	EPE	O2S-S-C10	3.66	110.03	106.91
8	D	1000	EPE	O1S-S-C10	4.10	110.41	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	FRU	1	0
8	B	1000	EPE	3	0
8	D	1000	EPE	2	0
8	F	1000	EPE	3	0
8	H	1000	EPE	2	0
6	I	2002	SO4	1	0
8	J	1000	EPE	2	0
3	K	1000	FRU	1	0
8	L	1000	EPE	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	537/537 (100%)	-0.07	5 (0%)	85	84	14, 27, 43, 56	0
1	C	537/537 (100%)	-0.09	9 (1%)	73	69	17, 31, 45, 60	0
1	E	537/537 (100%)	-0.01	11 (2%)	68	64	16, 30, 45, 61	0
1	G	537/537 (100%)	-0.03	11 (2%)	68	64	17, 31, 46, 59	0
1	I	537/537 (100%)	-0.09	7 (1%)	79	77	15, 29, 46, 59	0
1	K	537/537 (100%)	0.01	11 (2%)	68	64	19, 33, 51, 64	0
2	B	146/149 (97%)	0.21	4 (2%)	58	54	19, 32, 55, 62	0
2	D	146/149 (97%)	0.05	3 (2%)	67	63	20, 33, 50, 55	0
2	F	146/149 (97%)	0.18	6 (4%)	41	36	20, 33, 49, 57	0
2	H	146/149 (97%)	0.38	8 (5%)	29	24	22, 31, 51, 56	0
2	J	146/149 (97%)	0.13	4 (2%)	58	54	18, 27, 48, 55	0
2	L	146/149 (97%)	0.12	3 (2%)	67	63	18, 31, 48, 53	0
All	All	4098/4116 (99%)	0.00	82 (2%)	68	64	14, 30, 47, 64	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	121	SER	8.7
1	K	226	PRO	7.6
1	K	224	GLY	7.5
2	L	121	SER	7.1
1	I	226	PRO	6.8
1	E	224	GLY	6.8
1	G	226	PRO	6.3
1	K	439	ASN	6.0
2	J	119	LYS	6.0
1	A	226	PRO	5.8
1	G	224	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
2	F	121	SER	5.6
1	I	224	GLY	5.6
2	H	65	ALA	5.5
1	E	226	PRO	5.4
2	D	121	SER	5.2
1	E	213	PHE	4.9
2	B	121	SER	4.4
1	A	224	GLY	4.2
2	H	119	LYS	4.0
2	J	121	SER	3.9
1	K	213	PHE	3.8
2	L	119	LYS	3.8
1	K	381	ASP	3.6
1	I	213	PHE	3.5
1	E	225	GLU	3.5
1	C	227	ASN	3.5
1	C	226	PRO	3.4
1	K	437	ARG	3.3
1	E	439	ASN	3.3
1	G	439	ASN	3.3
2	B	119	LYS	3.2
2	H	120	GLY	3.2
2	H	64	ALA	3.1
1	G	541	SER	3.1
1	G	404	VAL	3.1
1	G	225	GLU	3.0
1	K	223	PHE	3.0
1	A	437	ARG	2.9
1	K	379	VAL	2.9
1	C	439	ASN	2.9
1	C	213	PHE	2.9
2	F	119	LYS	2.8
1	I	381	ASP	2.8
1	E	346	GLN	2.8
1	G	381	ASP	2.8
2	H	61	ASN	2.8
1	E	229	ILE	2.7
1	C	437	ARG	2.7
1	C	224	GLY	2.6
2	F	122	LYS	2.6
1	I	441	ASN	2.6
2	D	119	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	120	GLY	2.5
2	H	62	PRO	2.5
1	C	438	GLN	2.5
1	E	397	LEU	2.4
2	F	116	GLU	2.4
1	G	453	ARG	2.4
1	K	438	GLN	2.4
2	F	66	TRP	2.3
1	E	228	GLU	2.3
1	K	511	LYS	2.3
1	G	438	GLN	2.3
2	D	120	GLY	2.3
2	H	19	LYS	2.3
2	L	122	LYS	2.3
1	K	380	ARG	2.2
1	C	157	GLN	2.2
1	A	225	GLU	2.2
1	E	385	ALA	2.2
1	I	346	GLN	2.2
1	E	438	GLN	2.2
1	G	213	PHE	2.2
1	G	351	ARG	2.2
2	B	64	ALA	2.2
2	B	122	LYS	2.1
1	A	213	PHE	2.0
2	J	64	ALA	2.0
1	I	380	ARG	2.0
2	J	56	LYS	2.0
1	C	380	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	C	1001	14/15	0.95	0.16	0.94	21,22,25,26	0
4	NAG	G	1001	14/15	0.96	0.15	0.83	21,22,24,24	0
4	NAG	E	1001	14/15	0.95	0.16	0.14	23,25,27,31	0
4	NAG	A	1001	14/15	0.96	0.14	0.14	15,18,21,21	0
4	NAG	K	1001	14/15	0.93	0.14	-0.19	20,22,24,24	0
4	NAG	I	1001	14/15	0.96	0.14	-0.45	21,22,23,24	0
4	BMA	K	1005	11/12	0.73	0.28	-	42,43,44,45	0
4	MAN	I	1004	11/12	0.95	0.12	-	34,35,36,38	0
5	NAG	C	2000	14/15	0.91	0.20	-	33,36,38,40	0
5	NAG	C	2001	14/15	0.83	0.28	-	42,44,45,46	0
4	NAG	K	1002	14/15	0.94	0.13	-	24,26,28,31	0
4	MAN	I	1006	11/12	0.83	0.20	-	40,42,43,43	0
5	NAG	K	2001	14/15	0.76	0.43	-	43,44,46,46	0
4	BMA	C	1003	11/12	0.94	0.10	-	35,37,39,41	0
5	NAG	G	2000	14/15	0.91	0.15	-	31,34,37,37	0
4	BMA	G	1005	11/12	0.73	0.22	-	40,41,42,43	0
5	NAG	K	2000	14/15	0.92	0.17	-	32,35,38,39	0
5	NAG	E	2000	14/15	0.89	0.21	-	34,37,40,41	0
4	NAG	E	1002	14/15	0.90	0.28	-	33,35,37,39	0
4	BMA	I	1003	11/12	0.95	0.13	-	30,32,34,36	0
4	MAN	E	1006	11/12	0.79	0.43	-	51,52,52,53	0
4	NAG	A	1002	14/15	0.96	0.16	-	22,23,25,28	0
5	NAG	A	2001	14/15	0.89	0.22	-	40,42,43,43	0
4	MAN	G	1006	11/12	0.79	0.18	-	41,42,43,43	0
4	MAN	C	1006	11/12	0.83	0.18	-	44,45,45,46	0
4	NAG	I	1002	14/15	0.94	0.18	-	24,26,27,28	0
4	BMA	C	1005	11/12	0.82	0.21	-	43,45,45,46	0
5	NAG	E	2001	14/15	0.68	0.36	-	44,45,46,46	0
4	MAN	K	1004	11/12	0.91	0.16	-	39,40,41,42	0
5	NAG	G	2001	14/15	0.79	0.23	-	39,41,43,43	0
4	MAN	G	1004	11/12	0.94	0.13	-	38,38,39,40	0
4	BMA	A	1003	11/12	0.97	0.11	-	30,32,34,35	0
4	BMA	E	1005	11/12	0.86	0.34	-	47,48,49,49	0
4	MAN	K	1006	11/12	0.80	0.22	-	44,46,47,47	0
4	BMA	K	1003	11/12	0.94	0.12	-	33,35,37,39	0
4	BMA	A	1005	11/12	0.84	0.22	-	37,39,40,40	0
4	MAN	A	1006	11/12	0.84	0.21	-	41,42,43,43	0
4	BMA	I	1005	11/12	0.85	0.19	-	37,38,39,40	0
4	NAG	C	1002	14/15	0.95	0.15	-	27,28,30,33	0
5	NAG	A	2000	14/15	0.90	0.17	-	32,36,37,38	0
4	NAG	G	1002	14/15	0.95	0.13	-	25,26,28,30	0
4	BMA	E	1003	11/12	0.93	0.17	-	41,43,45,45	0
4	MAN	E	1004	11/12	0.92	0.28	-	46,47,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	BMA	G	1003	11/12	0.96	0.10	-	33,35,37,38	0
4	MAN	C	1004	11/12	0.95	0.12	-	38,39,39,42	0
4	MAN	A	1004	11/12	0.96	0.12	-	35,36,36,39	0
5	NAG	I	2000	14/15	0.86	0.20	-	33,36,38,39	0
5	NAG	I	2001	14/15	0.75	0.33	-	41,42,45,45	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	EPE	D	1000	15/15	0.82	0.30	8.85	43,45,51,52	0
8	EPE	F	1000	15/15	0.77	0.33	7.55	43,46,51,52	0
8	EPE	J	1000	15/15	0.85	0.28	6.96	40,42,48,48	0
8	EPE	L	1000	15/15	0.86	0.32	6.61	45,46,50,50	0
8	EPE	H	1000	15/15	0.87	0.29	5.28	46,47,52,52	0
8	EPE	B	1000	15/15	0.88	0.24	3.04	34,37,44,44	0
3	FRU	E	1000	12/12	0.97	0.15	1.60	21,22,22,23	0
3	FRU	G	1000	12/12	0.97	0.15	0.29	18,21,22,22	0
3	FRU	I	1000	12/12	0.97	0.14	0.26	22,23,24,24	0
3	FRU	A	1000	12/12	0.97	0.14	-0.17	18,19,19,20	0
3	FRU	C	1000	12/12	0.97	0.13	-0.18	20,20,21,21	0
3	FRU	K	1000	12/12	0.95	0.14	-0.28	22,23,23,23	0
6	SO4	B	1001	5/5	0.98	0.10	-	45,45,45,45	0
7	NAG	K	3000	14/15	0.93	0.15	-	33,35,36,36	0
6	SO4	I	2002	5/5	0.96	0.17	-	49,49,50,50	0
6	SO4	A	2002	5/5	0.97	0.15	-	43,43,44,44	0
7	NAG	C	3000	14/15	0.91	0.13	-	33,35,38,39	0
7	NAG	E	3000	14/15	0.90	0.20	-	33,36,37,37	0
6	SO4	E	2002	5/5	0.94	0.25	-	56,57,57,57	0
6	SO4	C	2002	5/5	0.94	0.16	-	54,54,55,55	0
7	NAG	G	3000	14/15	0.85	0.16	-	32,35,37,37	0
6	SO4	G	2002	5/5	0.87	0.22	-	63,64,64,64	0
7	NAG	A	3000	14/15	0.93	0.12	-	34,37,38,39	0
6	SO4	K	2002	5/5	0.96	0.16	-	51,51,52,52	0
7	NAG	I	3000	14/15	0.95	0.15	-	30,33,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.